THEOCHEM, VOLUME 54 (1989)

(*Journal of Molecular Structure, Vol. 185*)

AUTHOR INDEX

Balaban, A.T., 139
Balasubramanian, K., 229
Barysz, M., 95
Bonchev, D., 155
Brocas, J., 139

Dias, J.R., 57

Epiotis, N.D., 83

García-Bach, M.A., 275, 287

Hosoya, H., 123
Hu, J.N., 203

King, R.B., 15
Kirby, E.C., 39
Klein, D.J., 275, 287

Nikolić, S., 95
Nowakowski, J., 95

Plavšić, D., 249

Randić, M., 95, 249
Rouvray, D.H., 1, 187

Schaad, L.J., 203
Seitz, W.A., 275
Slanina, Z., 217

Trinajstić, N., 95, 249
Tsuchiya, A., 123

Valenti, R., 287

Živković, T.P., 169

THEOCHEM, VOLUME 54 (1989)

(*Journal of Molecular Structure, Vol. 185*)

SUBJECT INDEX

Aromaticity
Aromaticity in polycyclic conjugated hydrocarbon dianions, 249

Benzenoids
A theoretical study of C_{60} benzenoids, 57

Cayley
The pioneering contributions of Cayley and Sylvester to the mathematical description of chemical structure, 1
Centre of a chemical structure
The concept for the centre of a chemical structure and its applications, 155
Chemical graphs
Do chemical graphs have a natural order? Some regularities of a "compacted maximal adjacency code", 39
Chemical structure
The pioneering contributions of Cayley and Sylvester to the mathematical description of chemical structure, 1
Claus structures
On the importance of Claus structures, 169
Cluster expansions
Variational localized-site cluster expansions. Part 16. Excitations, 275
Comb polyenes
Analysis of the π-electronic structure of infinitely large networks. Part 2. Linear and comb polyenes with bond alternation, 123
Compacted maximal adjacency code
Do chemical grpahs have a natural order? Some regularities of a "compacted maximal adjacency code", 39
Computer design
Some aspects of mathematical chemistry of equilibrium and rate processes: steps towards a completely non-empirical computer design of syntheses, 217

Dianions
Aromaticity in polycyclic conjugated hydrocarbon dianions, 249

Edge-colorings of graphs
Applications of edge-colorings of graphs and characteristic polynomials to spectroscopy and quantum chemistry, 229
π-Electronic structure
Analysis of the π-electronic structure of infinitely large networks. Part 2. Linear and comb polyenes with bond alternation, 123
Equilibrium
Some aspects of mathematical chemistry of equilibrium and rate processes: steps towards a completely non-empirical computer design of syntheses, 217

Herdon–Simpson model
Covalent excitations of a polyphene polymer via a Herndon–Simpson model, 287

Isospectral graphs
Isospectral graphs revisited, 95

Linear polyenes
Analysis of the π-electronic structure of infinitely large networks. Part 2. Linear and comb polyenes with bond alternation, 123

Metal carbonyl clusters
Metal cluster topology. Part 8. Six-vertex polyhedral metal carbonyl clusters and their skeletal rearrangements, 15
Metal cluster
Metal cluster topology. Part 8. Six-vertex polyhedral metal carbonyl clusters and their skeletal rearrangements, 15

Natural order
Do chemical graphs have a natural order? Some regularities of a "compacted maximal adjacency code", 39
Networks
Analysis of the π-electronic structure of infinitely large networks. Part 2. Linear and comb polyenes with bond alternation, 123

Organometallic bonding
Three faces of organometallic bonding, 83

Pioneering contributions
The pioneering contributions of Cayley and Sylvester to the mathematical description of chemical structure, 1
Polynomials
Applications of edge-colorings of graphs and characteristic polynomials to spectroscopy and quantum chemistry, 229
Polyphene polymer
Covalent excitations of a polyphene polymer via a Herndon–Simpson model, 287

Quantum chemistry
Applications of edge-colorings of graphs and characteristic polynomials to spectroscopy and quantum chemistry, 229

Rate processes
Some aspects of mathematical chemistry of equilibrium and rate processes: steps towards a completely non-empirical computer design of syntheses, 217
Reaction graphs
Modes of rearrangements and reaction graphs for XeF_6, 139

Schrödinger equation

The Schrödinger equation in generalized coordinates, 203
Sylvester
The pioneering contributions of Cayley and Sylvester to the mathematical description of chemical structure, 1
Spectroscopy
Applications of edge-colorings of graphs and characteristic polynomials to spectroscopy and quantum chemistry, 229

Topological indices
The limits of applicability of topological indices, 187
Topology
Metal cluster topology. Part 8. Six-vertex polyhedral metal carbonyl clusters and their skeletal rearrangements, 15

XeF_6
Modes of rearrangements and reaction graphs for XeF_6, 139